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Topological Susceptibility to the One-Loop Order in Chiral Perturbation Theory

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Abstract

We derive the topological susceptibility to the one-loop order in the chiral effective theory of QCD, for an arbitrary number of flavors.

I. INTRODUCTION

In Quantum Chromodynamics (QCD), the topological susceptibility (χ_t) is the most crucial quantity to measure the topological charge fluctuation of the QCD vacuum, which plays an important role in breaking the $U_A(1)$ symmetry. Theoretically, χ_t is defined as

$$\chi_t = \int d^4x \, \langle \rho(x)\rho(0) \rangle \,, \tag{1}$$

where

$$\rho(x) = \frac{1}{32\pi^2}\epsilon_{\mu\nu\lambda\sigma}\mathrm{tr}[F_{\mu\nu}(x)F_{\lambda\sigma}(x)], \tag{2}$$

is the topological charge density expressed in term of the matrix-valued field tensor $F_{\mu\nu}$. With mild assumptions, Witten [1] and Veneziano [2] obtained a relationship between the topological susceptibility in the quenched approximation and the mass of η' meson (flavor singlet) in unquenched QCD with N_f degenerate flavors, namely,

$$\chi_t(\text{quenched}) = \frac{F_\pi^2 m_{\eta'}^2}{2N_f},$$

where $F_\pi \simeq 93$ MeV, the decay constant of pion. This implies that the mass of η' is essentially due to the axial anomaly relating to non-trivial topological charge fluctuations, which can turn out to be nonzero even in the chiral limit, unlike those of the (non-singlet) approximate Goldstone bosons.

Using the Chiral Perturbation Theory (ChPT), Leutwyler and Smilga [3, 4] obtained the following relations in the chiral limit

$$\chi_t = \Sigma\left(\frac{1}{m_u} + \frac{1}{m_d}\right)^{-1}, \quad (N_f = 2), \tag{3}$$

$$\chi_t = \Sigma\left(\frac{1}{m_u} + \frac{1}{m_d} + \frac{1}{m_s}\right)^{-1}, \quad (N_f = 3), \tag{4}$$

where m_u, m_d, and m_s are the quark masses, and Σ is the chiral condensate. This implies that in the chiral limit ($m_u \to 0$) the topological susceptibility is suppressed due to internal quark loops. Most importantly, (3) and (4) provide a viable way to extract Σ from χ_t in the chiral limit.

From (1), one obtains

$$\chi_t = \frac{\langle Q_t^2 \rangle}{\Omega}, \quad Q_t \equiv \int d^4x \rho(x), \tag{5}$$

where Ω is the volume of the system, and Q_t is the topological charge (which is an integer for QCD). Thus, one can determine χ_t by counting the number of gauge configurations for each topological sector. Furthermore, we can also obtain the second normalized cumulant

$$c_4 = -\frac{1}{\Omega}\left[\langle Q_t^4\rangle - 3\langle Q_t^2\rangle^2\right], \tag{6}$$

which is related to the leading anomalous contribution to the $\eta' - \eta'$ scattering amplitude in QCD, as well as the dependence of the vacuum energy on the vacuum angle θ. (For a recent review, see for example, Ref. [5] and references therein.)

However, for lattice QCD, it is difficult to extract $\rho(x)$ and Q_t unambiguously from the gauge link variables, due to their rather strong fluctuations.

To circumvent this difficulty, one may consider the Atiyah-Singer index theorem [6]

$$Q_t = n_+ - n_- = \mathrm{index}(\mathcal{D}), \tag{7}$$

where $n_\pm$ is the number of zero modes of the massless Dirac operator $\mathcal{D} \equiv \gamma_\mu(\partial_\mu + igA_\mu)$ with $\pm$ chirality. Since $\mathcal{D}$ is anti-Hermitian and chirally symmetric, its nonzero eigenmodes must come in complex conjugate pairs with zero chirality. Thus one can obtain the identity

$$n_+ - n_- = m\int d^4x \ \mathrm{tr}[\gamma_5(\mathcal{D}+m)^{-1}(x,x)], \tag{8}$$

by spectral decomposition, where the nonzero modes drop out due to zero chirality. In view of (7) and (8), one can regard $\rho_t(x) \equiv m_q \mathrm{tr}[\gamma_5(\mathcal{D}+m_q)^{-1}(x,x)]$ as topological charge density, to replace $\rho(x)$ in the measurement of χ_t.

Recently, the topological susceptibility and the second normalized cumulant have been measured in unquenched lattice QCD with exact chiral symmetry, for $N_f = 2$ and $N_f = 2+1$ lattice QCD with overlap fermion in a fixed topology [7, 8], and $N_f = 2+1$ lattice QCD with domain-wall fermion [9]. The results of topological susceptibility turn out in good agreement with the Leutwyler-Smilga relation, with the values of the chiral condensate as follows.

$$\begin{aligned}
\Sigma^{\overline{\mathrm{MS}}}(2\ \mathrm{GeV}) &= [245(5)(12)\ \mathrm{MeV}]^3, \quad (N_f = 2), \quad \text{Ref. [7]}, \\
\Sigma^{\overline{\mathrm{MS}}}(2\ \mathrm{GeV}) &= [253(4)(6)\ \mathrm{MeV}]^3, \quad (N_f = 2+1), \quad \text{Ref. [8]}, \\
\Sigma^{\overline{\mathrm{MS}}}(2\ \mathrm{GeV}) &= [259(6)(9)\ \mathrm{MeV}]^3, \quad (N_f = 2+1), \quad \text{Ref. [9]}.
\end{aligned}$$

These results assure that lattice QCD with exact chiral symmetry is the proper framework to tackle the strong interaction physics with topologically non-trivial vacuum fluctuations.

Obviously, the next task for unquenched lattice QCD with exact chiral symmetry is to determine the second normalized cumulant c_4 to a good precision, and to address the question how the vacuum energy depends on the vacuum angle θ and related problems. Theoretically, it is interesting to obtain an analytic expression of c_4 in ChPT, as well as to extend the Leutwyler-Smilga relation to the one-loop order. In this paper, we derive the topological susceptibility to the one-loop order in ChPT, for an arbitrary number of flavors.

The outline of this paper is as follows. In Section 2, we review the derivation of topological susceptibility χ_t at the tree level of ChPT, and also derive the second normalized cumulant c_4 at the tree level, and discuss its implications. In Section 3, we derive χ_t up to the one-loop order in ChPT for an arbitrary number of flavors. In Section 4, we conclude with some remarks, and also present the case of 2+1 flavors, in which only the one-loop corrections due to the u and d quarks are incorporated. In the Appendix, we present a heuristic derivation of the counterpart of the Leutwyler-Smilga relation in lattice QCD with exact chiral symmetry.

II. TOPOLOGICAL SUSCEPTIBILITY AT THE TREE LEVEL OF CHPT

Before we proceed to derive χ_t to the one-loop order in ChPT, it is instructive for us to recap the derivation of χ_t at the tree level [3, 4].

The leading terms of the effective chiral lagrangian for QCD with N_f flavor at $\theta = 0$ [10] are the kinetic term and the symmetry breaking term,

$$\mathcal{L}^{(2)} = \mathcal{L}^{(2)}_{\text{eff}} + \mathcal{L}^{(2)}_{\text{s.b.}} = \frac{F_\pi^2}{4}\text{Tr}(\partial_\mu U \partial^\mu U^\dagger) + \frac{\Sigma}{2}\text{Tr}(\mathcal{M}U^\dagger + U\mathcal{M}^\dagger), \tag{9}$$

where $U(x) = \exp\{2i\phi^a(x)t^a/F_\pi\}$ is a group element of $SU(N_f)$, $\mathcal{M}$ is the quark mass matrix, F_π is the pion decay constant, and $\Sigma = \langle\bar{\psi}\psi\rangle_{\text{vac}}$ is the chiral condensate of the QCD vacuum.

On the other hand, the partition function of QCD in the θ vacuum can be written as

$$Z_{N_f}(\theta) = \sum_Q e^{-iQ\theta} Z_Q, \tag{10}$$

where

$$\begin{aligned} Z_Q &= \int [dA_\mu] e^{-S_G[A_\mu]} \det\left(\gamma_\mu D_\mu + \frac{1-\gamma^5}{2}\mathcal{M} + \frac{1+\gamma^5}{2}\mathcal{M}^\dagger\right) \\ &= \int [dA_\mu] e^{-S_G[A_\mu]} \prod_k \det(\lambda_k^2 + \mathcal{M}^\dagger\mathcal{M}) \cdot \begin{cases} \det(\mathcal{M}^\dagger)^Q, & Q > 0, \\ \det(\mathcal{M})^{-Q}, & Q < 0, \end{cases} \end{aligned}$$

where S_G is the action of the gauge field, and λ_k's are non-zero eigenvalues of the massless Dirac operator $\gamma_\mu D_\mu$ in the gauge background. Thus the physical vacuum angle on which all physical quantities depend is $\theta_{\rm phys} = \theta + \arg\det(\mathcal{M})$ rather than θ. Also, the θ-dependence of $Z_{N_f}(\theta)$ always enters through the combinations $\mathcal{M}e^{i\theta/N_f}$ and $\mathcal{M}^\dagger e^{-i\theta/N_f}$. It follows that for $\theta \neq 0$, the symmetry breaking term in the chiral effective lagrangian can be written as

$$\mathcal{L}^{(2)}_{\rm s.b.} = \Sigma \ \mathrm{Re}\left[\mathrm{Tr}(\mathcal{M}e^{i\theta/N_f}U^\dagger)\right]. \tag{11}$$

Defining the vacuum energy density

$$\epsilon_{\rm vac}(\mathcal{M},\theta) = -\frac{1}{\Omega}\log Z_{N_f}(\theta), \tag{12}$$

then the topological susceptibility χ_t (5) and the second normalized culmulant c_4 (6) can be expressed as

$$\chi_t = \left.\frac{\partial^2\epsilon_{\rm vac}(\mathcal{M},\theta)}{\partial^2\theta}\right|_{\theta=0}, \tag{13}$$

$$c_4 = \left.\frac{\partial^4\epsilon_{\rm vac}(\mathcal{M},\theta)}{\partial^4\theta}\right|_{\theta=0}. \tag{14}$$

For small quark masses ($L \ll m_\pi^{-1}$), the unitary matrix U does not depend on x_μ. Thus only the symmetry-breaking term survives in (9), and the partition function becomes

$$Z_{N_f}(\theta) = \int dU \exp\left\{\Omega\ \Sigma\ \mathrm{Re}\left[\mathrm{Tr}(\mathcal{M}e^{i\theta/N_f}U^\dagger)\right]\right\}, \tag{15}$$

where $\Omega = L^3T$ is the space-time volume. Without loss of generality, the unitary matrix U can be taken to be diagonal

$$U = \mathrm{diag}\left(e^{i\alpha_1}, e^{i\alpha_2}, \ldots, e^{i\alpha_{N_f}}\right), \quad \sum_{j=1}^{N_f}\alpha_j = 0,$$

where the last constraint follows from the unitarity of U. Also, we can choose the mass matrix to be diagonal $\mathcal{M} = \mathrm{diag}(m_1, \ldots, m_{N_f})$. Then we have

$$\mathrm{Re}\left[\mathrm{Tr}(\mathcal{M}e^{i\theta/N_f}U^\dagger)\right] = \sum_j m_j\cos\phi_j,$$

where $\phi_j = \theta/N_f - \alpha_j$, and $\sum_j \phi_j = \theta$.

Now, we consider a sufficiently large volume Ω satisfying $m_j\Sigma\Omega \gg 1$, then the group integral in the partition function (15) is largely due to the U which minimizes the minus exponent of the integrand, i.e.,

$$\min_U\left\{-\mathrm{Re}\left[\mathrm{Tr}(\mathcal{M}e^{i\theta/N_f}U^\dagger)\right]\right\} = \min_\phi\left\{-\sum_{j=1}^{N_f}m_j\cos\phi_j\right\}, \quad \sum_{j=1}^{N_f}\phi_j = \theta. \tag{16}$$

For $N_f = 2$, this amounts to minimize the function

$$-m_1 \cos(\phi_1) - m_2 \cos(\theta - \phi_1),$$

where the constraint $\phi_1 + \phi_2 = \theta$ has been used. A simple calculation gives the minimum,

$$-\sqrt{m_1^2 + m_2^2 + 2m_1 m_2 \cos\theta}.$$

Thus the partition function is

$$Z_{N_f}(\theta) = Z_0 \exp\left\{\Omega\Sigma\sqrt{m_1^2 + m_2^2 + 2m_1 m_2 \cos\theta}\right\}, \quad m\Sigma\Omega \gg 1,$$

which gives the vacuum energy

$$\epsilon_{\rm vac}(\theta) = \epsilon_0 - \Sigma\sqrt{m_u^2 + m_d^2 + 2m_u m_d \cos\theta},$$

where ϵ_0 is the additive normalization constant corresponding the normalization factor Z_0 in the partition function. From (17), we obtain the topological susceptibility

$$\chi_t = \left.\frac{\partial^2 \epsilon_{\rm vac}}{\partial\theta^2}\right|_{\theta=0} = \Sigma\frac{m_u m_d}{m_u + m_d}. \tag{17}$$

Furthermore, the second normalized cumulant is

$$c_4 = \left.\frac{\partial^4 \epsilon_{\rm vac}}{\partial\theta^4}\right|_{\theta=0} = -\Sigma\frac{m_u m_d}{m_u + m_d} + 3\Sigma\frac{m_u^2 m_d^2}{(m_u + m_d)^3} = -\Sigma\left(\frac{1}{m_u^3} + \frac{1}{m_d^3}\right)\left(\frac{m_u m_d}{m_u + m_d}\right)^4, \tag{18}$$

which has not been discussed explicitly in the literature. The vital observation is that the ratio of χ_t and c_4 is

$$\frac{c_4}{\chi_t} = -1 + \frac{3m_u m_d}{(m_u + m_d)^2}, \tag{19}$$

which goes to $-1/4$ in the isospin limit $m_u = m_d$. This seems to rule out the dilute instanton gas/liquid model [11, 12, 13] which predicts that $c_4/\chi_t = -1$. Moreover, recent numerical results of c_4/χ_t from quenched lattice QCD [14, 15, 16] and unquenched lattice QCD [8, 9] are consistent with the prediction of ChPT.

Next we turn to the case $N_f > 2$. Then there is no analytic solution to the minimization problem (16). However, for the purpose of obtaining the topological susceptibility, one may consider the limit of small θ (and ϕ_j's) because $U = \mathbb{I}$ gives the minimal vacuum energy at $\theta = 0$. Since χ_t only depends on the curvature of $\epsilon_{\rm vac}(\theta)$ around $\theta = 0$, this approximation

would give the exact result of χ_t (at the tree-level). To the order of θ^4, the minimization problem (16) becomes

$$\min_{\phi}\left\{-\sum_{j=1}^{N_f} m_j\cos\phi_j\right\} = \min_{\phi}\left\{\frac{1}{2}\sum_{j=1}^{N_f} m_j\phi_j^2 - \frac{1}{24}\sum_{j=1}^{N_f} m_j\phi_j^4\right\}, \quad \sum_{i=1}^{N_f}\phi_i = \theta.$$

Now introducing the Lagrange multiplier λ to incorporate the constraint $\sum_i \phi_i = \theta$, then the minimization problem amounts to solving the equation

$$\frac{\partial}{\partial\phi_i}\left[\frac{1}{2}\sum_{j=1}^{N_f} m_j\phi_j^2 - \frac{1}{24}\sum_{j=1}^{N_f} m_j\phi_j^4 - \lambda\left(\sum_{j=1}^{N_f}\phi_j - \theta\right)\right] = m_i\phi_i - \frac{1}{6}m_i\phi_i^3 - \lambda = 0.$$

Setting $\phi_i = a_1\frac{\lambda}{m_i} + a_3\left(\frac{\lambda}{m_i}\right)^3$ (where a_1 and a_3 are parameters), and using $\sum_i \phi_i = \theta$, we can solve for a_1 and a_3, and ϕ_i to the order of θ^3,

$$\phi_i = \frac{\bar{m}}{m_i}\theta + \frac{\theta^3}{6}\left[\left(\frac{\bar{m}}{m_i}\right)^3 - \left(\frac{\bar{m}}{m_i}\right)\sum_{j=1}^{N_f}\left(\frac{\bar{m}}{m_j}\right)^3\right] + \mathcal{O}(\theta^5).$$

where $\bar{m} \equiv \left(\sum_{i=1}^{N_f} m_i^{-1}\right)^{-1}$ is the "reduced mass" of the N_f quark flavors. Keeping the exponent of the partition function to the order of θ^4, we have

$$Z_{N_f}(\theta) = Z_0\exp\left\{-\Omega\Sigma\left(\sum_{j=1}^{N_f}\frac{1}{m_j}\right)^{-1}\frac{\theta^2}{2} + \Omega\Sigma\sum_{i=1}^{N_f} m_i^{-3}\left(\sum_{j=1}^{N_f}\frac{1}{m_j}\right)^{-4}\frac{\theta^4}{24} + \mathcal{O}(\theta^6)\right\}, \quad (20)$$

and the vacuum energy density is

$$\epsilon_{\mathrm{vac}}(\theta) = \epsilon_0 + \Sigma\left(\sum_{j=1}^{N_f}\frac{1}{m_j}\right)^{-1}\frac{\theta^2}{2} - \Sigma\sum_{i=1}^{N_f} m_i^{-3}\left(\sum_{j=1}^{N_f}\frac{1}{m_j}\right)^{-4}\frac{\theta^4}{24} + \mathcal{O}(\theta^6).$$

It follows that the topological susceptibility is

$$\chi_t = \left.\frac{\partial^2\epsilon_{\mathrm{vac}}}{\partial\theta^2}\right|_{\theta=0} = \Sigma\left(\sum_{j=1}^{N_f}\frac{1}{m_j}\right)^{-1}, \quad (21)$$

and

$$c_4 = \left.\frac{\partial^4\epsilon_{\mathrm{vac}}}{\partial\theta^4}\right|_{\theta=0} = -\Sigma\sum_{i=1}^{N_f} m_i^{-3}\left(\sum_{j=1}^{N_f}\frac{1}{m_j}\right)^{-4}, \quad (22)$$

which generalize Eqs. (17) and (18) to an arbitrary number of flavors. In particular, for $N_f = 3$,

$$\chi_t = \Sigma\left(\frac{1}{m_u} + \frac{1}{m_d} + \frac{1}{m_s}\right)^{-1}, \quad (23)$$

and

$$c_4 = -\Sigma \left(\frac{1}{m_u^3} + \frac{1}{m_d^3} + \frac{1}{m_s^3} \right) \left(\frac{1}{m_u} + \frac{1}{m_d} + \frac{1}{m_s} \right)^{-4}. \tag{24}$$

Nevertheless, these two formulas seem unnatural, since the strange quark is much heavier than the up and down quarks. Thus a plausible chiral limit is to take $m_{u,d} \to 0$, while keeping m_s fixed. Consequently, the condensate of the strange quark $\langle \bar{s}s \rangle$ must be different from Σ, and it should also enter this formula. In the Appendix, we present a heuristic derivation of the counterpart of (23) in lattice QCD with exact chiral symmetry, which takes into account of the difference between $\langle \bar{s}s \rangle$ and Σ, as given in Eq. (52).

III. TOPOLOGICAL SUSCEPTIBILITY TO THE ONE-LOOP ORDER OF CHPT

To the one-loop order of ChPT, one has to include $\mathcal{L}^{(4)}$ [10] at the tree level as well as the one-loop contributions of $\mathcal{L}^{(2)}$. In 1984, Gasser and Leutwyler [10] considered the low-energy expansion, where both p and $\mathcal{M}$ are assumed to be small but $\mathcal{M}/p^2$ can have a finite value, such that the value of M_π^2/p^2 can be fixed. In this case, the external sources $a_\mu(x)$ and $p(x)$ can be counted as order of Φ, and $v_\mu(x)$ and $s(x) - \mathcal{M}$ as order of Φ^2. Gasser and Leutwyler showed that at the one-loop order, the chiral effective action can be written as

$$W = W_t + W_u + W_A + \mathcal{O}(\Phi^6), \tag{25}$$

where W_t denotes the sum of tree diagrams and tadpole contributions (of order Φ^2), W_u the unitarity correction (of order Φ^3), and W_A the anomaly contribution (of order Φ^4). Because the θ dependence enters the Lagrangian only through $\mathcal{M}$, we can count χ_t as order of Φ^2, thus for the evaluation of topological susceptibility to the one-loop order, and it suffices to consider W_t only.

Moreover, Gasser and Leutwyler [10] showed that the pole terms due to the one-loop contributions of $\mathcal{L}^{(2)}$ can be absorbed by the low-energy coupling constants of $\mathcal{L}^{(4)}$, and W_t is given by [10]

$$\begin{aligned} W_t =& \sum_P \int d^4x \, \frac{F_\pi^2}{2} \left\{ \frac{1}{N_f} - \frac{M_P^2}{16\pi^2 F_\pi^2} \ln \frac{M_P^2}{\mu_{sub}^2} \right\} \sigma_{PP}^{\Delta} \\ &+ \sum_P \int d^4x \, \frac{F_\pi^2}{2} \left\{ \frac{N_f}{N_f^2 - 1} - \frac{M_P^2}{16\pi^2 F_\pi^2} \ln \frac{M_P^2}{\mu_{sub}^2} \right\} \sigma_{PP}^{\chi} + \int d^4x \mathcal{L}^{r(4)}, \end{aligned} \tag{26}$$

where M_P^2's are the squared meson masses, σ_{PP}^{Δ} corresponds to the kinetic term which can be dropped in the limit of small quark masses, σ_{PP}^{χ} corresponds to the symmetry breaking term,

$$\sigma_{PP}^{\chi} = \frac{1}{8}\mathrm{Tr}\left(\left\{\lambda_P, \lambda_P^\dagger\right\}(\chi^\dagger U + U^\dagger \chi)\right) - M_P^2 \ , \tag{27}$$

and $\mathcal{L}^{r(4)}$ is just $\mathcal{L}^{(4)}$ with renormalized low-energy coupling constants,

$$\begin{aligned}
\mathcal{L}^{r(4)} = & L_1^r \left\{\mathrm{Tr}[D_\mu U(D^\mu U)^\dagger]\right\}^2 + L_2^r \mathrm{Tr}\left[D_\mu U(D_\nu U)^\dagger\right]\mathrm{Tr}\left[D^\mu U(D^\nu U)^\dagger\right] \\
& + L_3^r \mathrm{Tr}\left[D_\mu U(D^\mu U)^\dagger D_\nu U(D^\nu U)^\dagger\right] \\
& + L_4^r \mathrm{Tr}\left[D_\mu U(D^\mu U)^\dagger\right]\mathrm{Tr}\left(\chi U^\dagger + U\chi^\dagger\right) \\
& + L_5^r \mathrm{Tr}\left[D_\mu U(D^\mu U)^\dagger(\chi U^\dagger + U\chi^\dagger)\right] + L_6^r\left[\mathrm{Tr}\left(\chi U^\dagger + U\chi^\dagger\right)\right]^2 \\
& + L_7^r\left[\mathrm{Tr}\left(\chi U^\dagger - U\chi^\dagger\right)\right]^2 + L_8^r \mathrm{Tr}\left(U\chi^\dagger U\chi^\dagger + \chi U^\dagger \chi U^\dagger\right) \\
& - iL_9^r \mathrm{Tr}\left[F_{\mu\nu}^R D^\mu U(D^\nu U)^\dagger + F_{\mu\nu}^L (D^\mu U)^\dagger D^\nu U\right] + L_{10}^r \mathrm{Tr}\left(U F_{\mu\nu}^L U^\dagger F_R^{\mu\nu}\right) \\
& + H_1^r \mathrm{Tr}\left(F_{\mu\nu}^R F_R^{\mu\nu} + F_{\mu\nu}^L F_L^{\mu\nu}\right) + H_2^r \mathrm{Tr}\left(\chi\chi^\dagger\right).
\end{aligned} \tag{28}$$

Here $\chi = 2(\Sigma/F_\pi^2)\mathcal{M} \equiv 2B_0\mathcal{M}$, λ_P's are the generators of $SU(N)$ in the physical basis, $\{L_i^r(\mu_{sub}), i = 1, \cdots, 10\}$ are renormalized low-energy coupling constants, and the last two contact terms (with couplings $H_1^r(\mu_{sub})$ and $H_2^r(\mu_{sub})$) are the counter terms required for renormalization of the one-loop diagrams.

For small quark masses ($L \ll m_\pi^{-1}$), the unitary matrix U does not depend on x_μ, thus the term involving σ_{PP}^{Δ} in (26) can be dropped.

Next we consider the term with σ_{PP}^{χ} in (26). Using the formula

$$\sum_P \left\{\lambda_P, \lambda_P^\dagger\right\} = \frac{4(N_f^2 - 1)}{N_f}\,\mathbb{1}, \tag{29}$$

we obtain its contribution to the chiral effective lagrangian,

$$\begin{aligned}
& \Sigma \mathrm{ReTr}(\mathcal{M}U^\dagger) - \frac{N_f F_\pi^2}{2(N_f^2-1)}\sum_P M_P^2 \\
& - \frac{\Sigma}{4F_\pi^2}\sum_P \mathrm{ReTr}\left(\left\{\lambda_P, \lambda_P^\dagger\right\}\mathcal{M}U^\dagger\right)\frac{M_P^2}{16\pi^2}\ln\frac{M_P^2}{\mu_{sub}^2} + \frac{M_P^4}{32\pi^2}\ln\frac{M_P^2}{\mu_{sub}^2}.
\end{aligned} \tag{30}$$

For small quark masses ($L \ll m_\pi^{-1}$), the unitary matrix U does not depend on x_μ, so only the sixth, seventh, and eighth terms in $\mathcal{L}^{r(4)}$ are relevant to the partition function. For $\theta \neq 0$,

θ enters the chiral effective lagrangian through the combinations $\mathcal{M}e^{i\theta/N_f}$ and $\mathcal{M}^\dagger e^{-i\theta/N_f}$. Thus these three potential terms can be written as

$$L_6^r\left[4B_0\mathrm{ReTr}(\mathcal{M}e^{i\theta/N_f}U^\dagger)\right]^2+L_7^r\left[i4B_0\mathrm{ImTr}(\mathcal{M}e^{i\theta/N_f}U^\dagger)\right]^2+8L_8^rB_0^2\mathrm{ReTr}\left[(\mathcal{M}e^{i\theta/N_f}U^\dagger)^2\right]. \tag{31}$$

Without loss of generality, we can take U and $\mathcal{M}$ to be diagonal,

$$\begin{aligned} U &= \mathrm{diag}\left(e^{i\alpha_1},e^{i\alpha_2},\ldots,e^{i\alpha_{N_f}}\right), \quad \sum_{j=1}^{N_f}\alpha_j=0, \\ \mathcal{M} &= \mathrm{diag}(m_1,\ldots,m_{N_f}), \end{aligned}$$

therefore the contributions of (30) and (31) become (dropping the terms without U dependence)

$$\begin{aligned} &\Sigma\sum_{j=1}^{N_f}m_j\cos\phi_j-\frac{\Sigma}{4F_\pi^2}\sum_P\sum_{j=1}^{N_f}\left\{\lambda_P,\lambda_P^\dagger\right\}_{jj}m_j\cos\phi_j\frac{M_P^2}{16\pi^2}\ln\frac{M_P^2}{\mu_{sub}^2} \\ &+\ 16B_0^2L_6^r\left(\sum_{j=1}^{N_f}m_j\cos\phi_j\right)^2-16B_0^2L_7^r\left(\sum_{j=1}^{N_f}m_j\sin\phi_j\right)^2+8B_0^2L_8^r\sum_{j=1}^{N_f}m_j^2\cos2\phi_j, \end{aligned}$$

where $\phi_j=\theta/N_f-\alpha_j$, and $\sum_j\phi_j=\theta$.

Again, we use small θ (small ϕ_j's) approximation and keep terms up to the order of ϕ_j^2, then the evaluation of the integral in the partition function in the limit $m_j\Omega\Sigma\gg1$ amounts to minimizing the generating functional

$$\begin{aligned} \min_\phi&\left[\frac{\Sigma}{2}\sum_{j=1}^{N_f}m_j\phi_j^2-\frac{\Sigma}{8F_\pi^2}\sum_P\sum_{j=1}^{N_f}\left\{\lambda_P,\lambda_P^\dagger\right\}_{jj}m_j\phi_j^2\frac{M_P^2}{16\pi^2}\ln\frac{M_P^2}{\mu_{sub}^2}\right. \\ &\left.+16B_0^2L_6^r\sum_{i=1}^{N_f}m_i\sum_{j=1}^{N_f}m_j\phi_j^2+16B_0^2L_7^r\left(\sum_{j=1}^{N_f}m_j\phi_j\right)^2+16B_0^2L_8^r\sum_{j=1}^{N_f}m_j^2\phi_j^2\right], \end{aligned} \tag{32}$$

with the constraint $\sum_j\phi_j=\theta$. We introduce the Lagrange multiplier λ to incorporate the constraint in finding the minimum. For simplicity, we define

$$\begin{aligned} A_j &\equiv \frac{\Sigma}{2}m_j-\frac{\Sigma}{8F_\pi^2}\sum_P\left\{\lambda_P,\lambda_P^\dagger\right\}_{jj}m_j\frac{M_P^2}{16\pi^2}\ln\frac{M_P^2}{\mu_{sub}^2}+16B_0^2\left(L_6^rm_j\sum_{i=1}^{N_f}m_i+L_8^rm_j^2\right), \\ B_j &\equiv 4B_0(L_7^r)^{1/2}m_j. \end{aligned}$$

Then the minimization problem amounts to solving the equation

$$\frac{\partial}{\partial\phi_i}\left[\sum_{j=1}^{N_f}A_j\phi_j^2+\left(\sum_{j=1}^{N_f}B_j\phi_j\right)^2-\lambda\left(\sum_{j=1}^{N_f}\phi_j-\theta\right)\right]=0,$$

which gives

$$A_i\phi_i + B_i\left(\sum_{j=1}^{N_f} B_j\phi_j\right) = \frac{\lambda}{2}. \tag{33}$$

Defining $(\mathbf{T})_{ij} \equiv 2A_i\delta_{ij} + 2B_iB_j$, (33) becomes

$$\sum_{j=1}^{N_f}(\mathbf{T})_{ij}\phi_j = \lambda, \quad i = 1,\ldots,N_f. \tag{34}$$

Thus we can obtain λ using the constraint

$$\theta = \sum_{j=1}^{N_f}\phi_j = \lambda\sum_{j=1}^{N_f}\sum_{i=1}^{N_f}(\mathbf{T}^{-1})_{ij} \;\Rightarrow\; \lambda = \theta\left[\sum_{j=1}^{N_f}\sum_{i=1}^{N_f}(\mathbf{T}^{-1})_{ij}\right]^{-1}. \tag{35}$$

Now multiplying Eq. (33) with ϕ_i and summing over i, we obtain

$$\min_{\phi}\left[\sum_{j=1}^{N_f} A_j\phi_j^2 + \left(\sum_{j=1}^{N_f} B_j\phi_j\right)^2\right] = \frac{\lambda\theta}{2}, \tag{36}$$

which can be used to simplify (32) to

$$\frac{\lambda\theta}{2} = \frac{\theta^2}{2}\left[\sum_{i,j=1}^{N_f}(\mathbf{T}^{-1})_{ij}\right]^{-1}, \tag{37}$$

where the last equality follows from (35). Finally, the partition function of QCD with N_f flavors to the one-loop order of ChPT in the limit $m\Sigma\Omega \gg 1$ is equal to

$$Z_{N_f}(\theta) = Z_0\exp\left\{\Omega\frac{\theta^2}{2}\left[\sum_{i,j=1}^{N_f}(\mathbf{T}^{-1})_{ij}\right]^{-1}\right\}, \tag{38}$$

and the vacuum energy density is

$$\epsilon_{\mathrm{vac}}(\theta) = \epsilon_0 + \frac{\theta^2}{2}\left[\sum_{i,j=1}^{N_f}(\mathbf{T}^{-1})_{ij}\right]^{-1}. \tag{39}$$

Thus the topological susceptibility to the one-loop order of ChPT is

$$\chi_t = \left.\frac{\partial^2\epsilon_{\mathrm{vac}}}{\partial\theta^2}\right|_{\theta=0} = \left[\sum_{i,j=1}^{N_f}(\mathbf{T}^{-1})_{ij}\right]^{-1}. \tag{40}$$

To simplify the expression of topological susceptibility, we rewrite the matrix $\mathbf{T}$ as

$$(\mathbf{T})_{ij} \equiv 2A_i\delta_{ij} + 2B_iB_j = \Sigma(\mathcal{M} + \mathbf{T}')_{ij}, \tag{41}$$

where

$$(\mathbf{T}')_{ij} = -\frac{1}{4F_\pi^2}\sum_P \left\{\lambda_P, \lambda_P^\dagger\right\}_{jj} m_j \delta_{ij} \frac{M_P^2}{16\pi^2} \ln \frac{M_P^2}{\mu_{sub}^2}$$
$$+K_6 \sum_{k=1}^{N_f} m_k m_j \delta_{ij} + K_8 m_j^2 \delta_{ij} + K_7 m_i m_j, \tag{42}$$

and

$$K_i \equiv \frac{32 B_0^2 L_i^r(\mu_{sub})}{\Sigma} = 32\left(\frac{\Sigma}{F_\pi^4}\right) L_i^r(\mu_{sub}). \tag{43}$$

Since the eigenvalues of the real and symmetric matrix $\mathcal{M}^{-1/2}\mathbf{T}'\mathcal{M}^{-1/2}$ are much less than one in the chiral limit, we can use the Taylor expansion

$$(\mathbb{1} + \mathcal{M}^{-1/2}\mathbf{T}'\mathcal{M}^{-1/2})^{-1} \simeq \mathbb{1} - \mathcal{M}^{-1/2}\mathbf{T}'\mathcal{M}^{-1/2} + \mathcal{O}(m^2),$$

and obtain

$$\begin{aligned}
\chi_t = \left[\sum_{i,j=1}^{N_f} (\mathbf{T}^{-1})_{ij}\right]^{-1} &\simeq \Sigma\bar{m}\left[1 + \bar{m}\sum_{i,j=1}^{N_f} \frac{(\mathbf{T}')_{ij}}{m_i m_j}\right] \\
&= \Sigma\bar{m}\left\{1 - \frac{1}{4F_\pi^2}\sum_P \sum_{j=1}^{N_f} \left\{\lambda_P, \lambda_P^\dagger\right\}_{jj} \left(\frac{\bar{m}}{m_j}\right) \frac{M_P^2}{16\pi^2} \ln \frac{M_P^2}{\mu_{sub}^2}\right. \\
&\qquad \left. +K_6 \sum_{i=1}^{N_f} m_i + N_f(N_f K_7 + K_8)\bar{m}\right\},
\end{aligned} \tag{44}$$

where $\bar{m} \equiv \left(\sum_{i=1}^{N_f} m_i^{-1}\right)^{-1}$, and all terms proportional to K_i^2 or $K_i K_j$ have been dropped. Equation (44) is the main result of this paper.

For $N_f = 2$, there are three mesons, π^+, π^0, and π^-. If we take their masses to be the same and use (29), we obtain

$$\begin{aligned}
\chi_t = \Sigma\left(\frac{1}{m_u} + \frac{1}{m_d}\right)^{-1} &\left[1 - \frac{3}{2F_\pi^2}\frac{M_\pi^2}{16\pi^2} \ln \frac{M_\pi^2}{\mu_{sub}^2} + K_6(m_u + m_d)\right. \\
&\left. + 2(2K_7 + K_8)\frac{m_u m_d}{m_u + m_d}\right].
\end{aligned} \tag{45}$$

Next we turn to the case $N_f = 3$. Taking the eight pseudoscalar mesons with non-degenerate masses, we obtain

$$\begin{aligned}
\chi_t = \Sigma\bar{m}&\left\{1 - \frac{1}{2F_\pi^2}\left[\sum_{i\neq j}\left(\frac{\bar{m}}{m_i} + \frac{\bar{m}}{m_j}\right)\frac{B_0(m_i + m_j)}{16\pi^2} \ln \frac{B_0(m_i + m_j)}{\mu_{sub}^2}\right.\right. \\
&\left. + \left(\frac{\bar{m}}{m_u} + \frac{\bar{m}}{m_d}\right)\frac{M_{\pi^0}^2}{16\pi^2} \ln \frac{M_{\pi^0}^2}{\mu_{sub}^2} + \frac{1}{3}\left(\frac{\bar{m}}{m_u} + \frac{\bar{m}}{m_d} + 4\frac{\bar{m}}{m_s}\right)\frac{M_\eta^2}{16\pi^2} \ln \frac{M_\eta^2}{\mu_{sub}^2}\right] \\
&\left. +K_6(m_u + m_d + m_s) + 3(3K_7 + K_8)\bar{m}\right\},
\end{aligned} \tag{46}$$

where $\bar{m} = \left(m_u^{-1} + m_d^{-1} + m_s^{-1}\right)^{-1}$, and $B_0 = \Sigma/F_\pi^2$.

IV. CONCLUDING REMARK

In this paper, we have derived the topological susceptibility to the one-loop order in ChPT, in the limit $m\Sigma\Omega \gg 1$, for $N_f = 2$ [Eq. (45)], $N_f = 3$ [Eq. (46)], and an arbitrary number of flavors N_f [Eq. (44)] respectively.

For $N_f = 3$, since the mass of the strange quark is much heavier than the masses of u and d quarks, it seems reasonable just to incorporate the one-loop corrections due to the u and d quarks. Then, for $N_f = 2+1$ (u and d quarks to the one-loop order, and s quark at the tree level), the topological susceptibility becomes

$$\chi_t = \Sigma\left\{ \left(\frac{1}{m_u} + \frac{1}{m_d}\right) \left[1 \; + \; \frac{3}{2F_\pi^2}\frac{M_\pi^2}{16\pi^2} \ln \frac{M_\pi^2}{\mu_{sub}^2} - K_6(m_u + m_d) \right.\right. \\ \left.\left. - \; 2(2K_7 + K_8)\frac{m_u m_d}{m_u + m_d}\right] + \frac{1}{m_s} \right\}^{-1}. \tag{47}$$

This supplements (46) for the case $N_f = 2+1$.

Now the trend of unquenched lattice QCD simulations is to include the charm quark. Thus it is also interesting to include the case $N_f = 2+1+1$, with both s and c quarks being kept at the tree level. Then the topological susceptibility is

$$\chi_t = \Sigma\left\{ \left(\frac{1}{m_u} + \frac{1}{m_d}\right) \left[1 \; + \; \frac{3}{2F_\pi^2}\frac{M_\pi^2}{16\pi^2} \ln \frac{M_\pi^2}{\mu_{sub}^2} - K_6(m_u + m_d) \right.\right. \\ \left.\left. - \; 2(2K_7 + K_8)\frac{m_u m_d}{m_u + m_d}\right] + \frac{1}{m_s} + \frac{1}{m_c} \right\}^{-1} \tag{48}$$

In view of the one-loop results of χ_t, [Eqs. (45), (46), (47), and (48)], it would be interesting to see whether the χ_t measured in lattice QCD with exact chiral symmetry would agree with the prediction of ChPT. Most importantly, these one-loop formulas provide a viable way to determine the low-energy constants F_π, L_6, L_7 and L_8, in addition to the chiral condensate Σ which has already been determined [7, 8, 9] using the formula of χ_t at the tree level (23).

Finally, we turn to the second normalized cumulant c_4. At this moment, we only have a formula of c_4 (22) at the tree level. For $N_f = 2$, the ratio $c_4/\chi_t = -1/4$ in the isospin limit ($m_u = m_d$) seems to rule out the instanton gas/liquid model which predicts that $c_4/\chi_t = -1$.

Obviously, it would be interesting to derive a formula of c_4 to the next (non-vanishing) order in ChPT.

Appendix

In this Appendix, we present a heuristic derivation of the relationship between topological susceptibility, chiral condensate, and the quark masses, for an arbitrary number of (non-degenerate) flavors, in the framework of lattice QCD with exact chiral symmetry. Our derivation generalizes that presented in Ref. [17] with degenerate flavors.

Consider the flavor-singlet pseudoscalar η'

$$\eta'(x) = \frac{1}{N_f} \sum_{i=1}^{N_f} \bar{q}_i(x)\gamma_5 q_i(x).$$

Its correlator at zero momentum is

$$\begin{aligned}
& G_{\eta'}(p=0) = \frac{1}{\Omega} \sum_{x,y} \langle \eta'(x) \eta'^{\dagger}(y) \rangle \\
= \; & \frac{1}{\Omega N_f^2} \sum_{x,y} \sum_{i,j=1}^{N_f} \langle \bar{q}_i(x)\gamma_5 q_i(x) \bar{q}_j(y)\gamma_5 q_j(y) \rangle \\
= \; & \frac{1}{\Omega Z N_f^2} \int [dU] \det D(m) e^{-S_g[U]} \times \\
& \left\{ \sum_{i=1}^{N_f} \mathrm{Tr}[(D_c+m_i)^{-1}\gamma_5 (D_c+m_i)^{-1}\gamma_5] - \left(\sum_{i=1}^{N_f} \mathrm{Tr}[(D_c+m_i)^{-1}\gamma_5] \right)^2 \right\} \\
= \; & \frac{1}{\Omega Z N_f^2} \int [dU] \det D(m) e^{-S_g[U]} \left\{ \sum_{i=1}^{N_f} \frac{1}{m_i} \mathrm{Tr}(D_c+m_i)^{-1} - \left[\sum_{i=1}^{N_f} \frac{1}{m_i}(n_+ - n_-) \right]^2 \right\}, \quad (49)
\end{aligned}$$

where $S_g[U]$ is the gauge action,

$$\begin{aligned}
\det D(m) &= \prod_{i=1}^{N_f} \det[(D_c+m_i)(1+rD_c)^{-1}], \\
Z &= \int [dU] \det D(m) e^{-S_g[U]},
\end{aligned}$$

and the identity

$$\mathrm{Tr}[(D_c+m)^{-1}\gamma_5 (D_c+m)^{-1}\gamma_5] = \frac{1}{m} \mathrm{Tr}(D_c+m)^{-1},$$

has been used in the last equality of (49). Here $D_c = D(1-rD)^{-1}$ is the chirally symmetric Dirac operator of a Ginsparg-Wilson Dirac operator D satisfying $D\gamma_5 + \gamma_5 D = 2rD\gamma_5 D$.

Now taking the thermodynamic limit ($\Omega \to \infty$), and then the chiral limit ($m_i \to 0$), (49) gives

$$G_{\eta'}(0) = \frac{1}{N_f^2} \left(\sum_{i=1}^{N_f} \frac{1}{m_i} \right) \left\{ \Sigma - \left(\sum_{i=1}^{N_f} \frac{1}{m_i} \right) \chi_t \right\}, \tag{50}$$

where

$$\begin{aligned} \Sigma &= \lim_{m_i \to 0} \lim_{\Omega \to \infty} \frac{1}{\Omega} \langle \mathrm{Tr}(D_c + m_i)^{-1} \rangle, \\ \chi_t &= \lim_{m_i \to 0} \lim_{\Omega \to \infty} \frac{1}{\Omega} \langle (n_+ - n_-)^2 \rangle. \end{aligned}$$

If η' stays massive, then its propagator $G_{\eta'} \propto m_{\eta'}^{-2}$ must be non-singular. This implies that the coefficient of the singular factor $\left(\sum_{i=1}^{N_f} \frac{1}{m_i} \right)$ in (50) behaves like $\mathcal{O}(m)$, i.e.,

$$\chi_t = \Sigma \left(\sum_{i=1}^{N_f} \frac{1}{m_i} \right)^{-1},$$

which agrees with the Leutwyler-Smilga relation.

For $N_f = 2 + 1$ with fixed m_s, (50) is modified to

$$G_{\eta'}(0) = \frac{1}{N_f^2} \left(\frac{2}{m_{u,d}} \right) \left\{ \Sigma \left(1 + \frac{m_{u,d}}{2m_s} \frac{\langle \bar{s}s \rangle}{\Sigma} \right) - \frac{2}{m_{u,d}} \left(1 + \frac{m_{u,d}}{2m_s} \right)^2 \chi_t \right\}, \tag{51}$$

where

$$\langle \bar{s}s \rangle \equiv \lim_{\Omega \to \infty} \frac{1}{\Omega} \langle \mathrm{Tr}(D_c + m_s)^{-1} \rangle.$$

In the limit $m_{u,d} \to 0$, the coefficient of the singular factor $2/m_{u,d}$ in (51) behaves like $\mathcal{O}(m_{u,d})$, i.e.,

$$\chi_t = \left(\frac{\Sigma}{m_u} + \frac{\Sigma}{m_d} + \frac{\langle \bar{s}s \rangle}{m_s} \right) \left(\frac{1}{m_u} + \frac{1}{m_d} + \frac{1}{m_s} \right)^{-2}, \tag{52}$$

which provides a more physical relationship (between χ_t, Σ, $\langle \bar{s}s \rangle$, and the quark masses) than the Leutwyler-Smilga relation (4), since it reduces to (4) only in the (unphysical) limit $\langle \bar{s}s \rangle = \Sigma$.

Now it is straightforward to generalize (52) to the case $N_f = 2 + 1 + 1$,

$$\chi_t = \left(\frac{\Sigma}{m_u} + \frac{\Sigma}{m_d} + \frac{\langle \bar{s}s \rangle}{m_s} + \frac{\langle \bar{c}c \rangle}{m_c} \right) \left(\frac{1}{m_u} + \frac{1}{m_d} + \frac{1}{m_s} + \frac{1}{m_c} \right)^{-2}, \tag{53}$$

where

$$\langle \bar{c}c \rangle \equiv \lim_{\Omega \to \infty} \frac{1}{\Omega} \langle \mathrm{Tr}(D_c + m_c)^{-1} \rangle.$$

It would be interesting to determine Σ, $\langle \bar{s}s \rangle$, and $\langle \bar{c}c \rangle$ with the data of χ_t in lattice QCD with exact chiral symmetry.

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